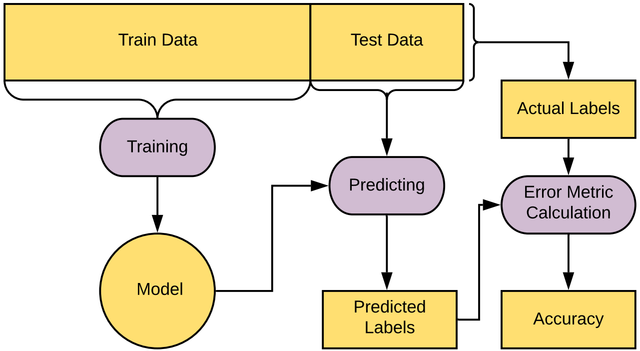
# Cross-Validation

Nipun Batra and teaching staff
IIT Gandhinagar

August 1, 2025

# Outline

# Our General Training Flow



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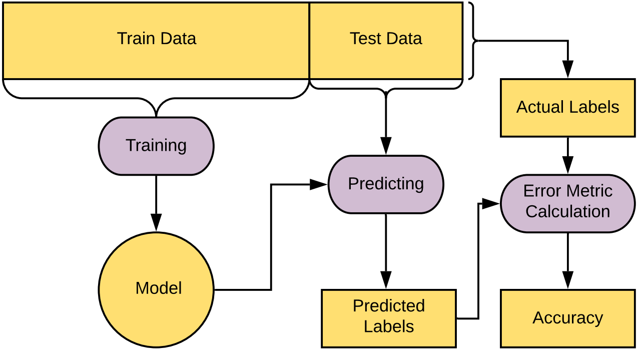

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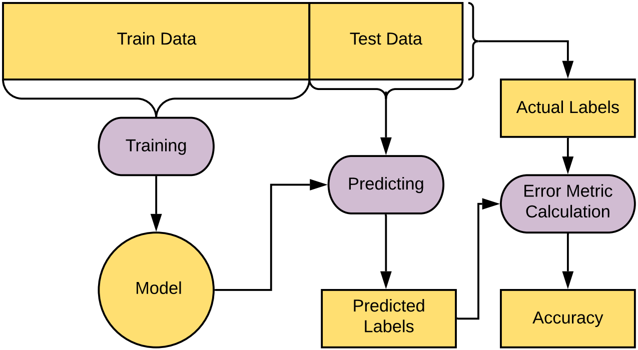


- Does not use the full dataset for training and does not test on the full dataset

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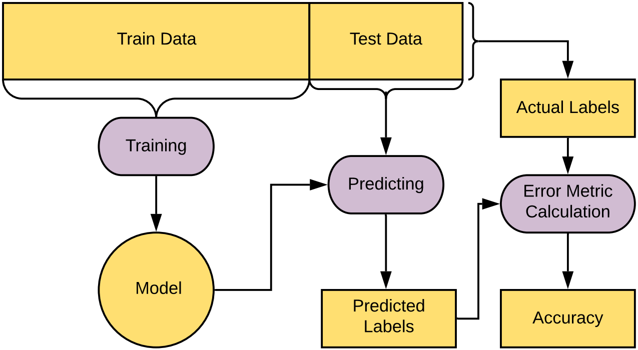


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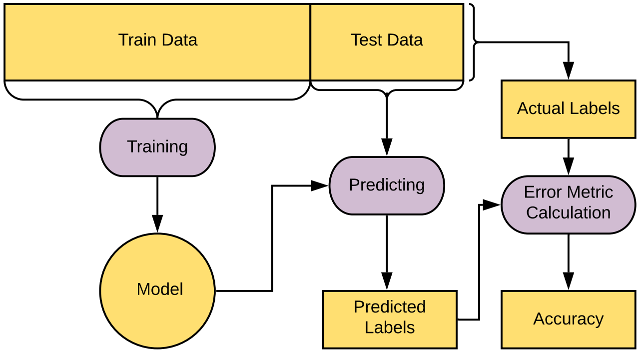


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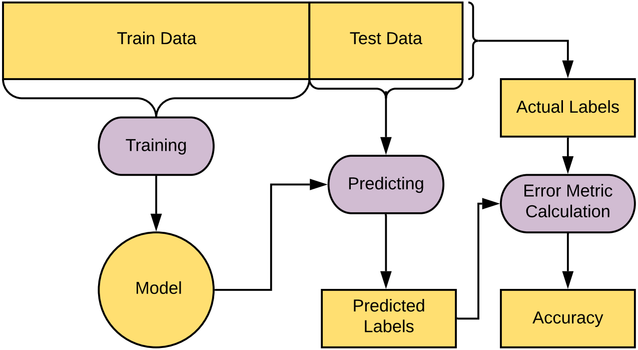


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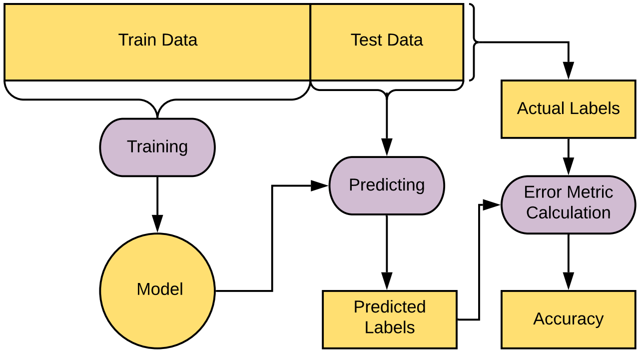


- Does not use the full dataset for training and does not test on the full dataset
- No way to optimize hyperparameters
- This simple train/test split has limitations we need to address

# Pop Quiz #1

**Question**

What are the main limitations of using only a single train/test split?

# Pop Quiz #2

## Question

What are the main limitations of using only a single train/test split?

# Pop Quiz #3

## Question

What are the main limitations of using only a single train/test split?

## Answer

# Pop Quiz #4

## Question

What are the main limitations of using only a single train/test split?

## Answer

- Does not utilize the full dataset for training

# Pop Quiz #5

## Question

What are the main limitations of using only a single train/test split?

## Answer

- Does not utilize the full dataset for training
- Cannot optimize hyperparameters systematically

# Pop Quiz #6

## Question

What are the main limitations of using only a single train/test split?

## Answer

- Does not utilize the full dataset for training
- Cannot optimize hyperparameters systematically
- Results depend on the particular split chosen

# Pop Quiz #7

## Question

What are the main limitations of using only a single train/test split?

## Answer

- Does not utilize the full dataset for training
- Cannot optimize hyperparameters systematically
- Results depend on the particular split chosen
- May not get reliable performance estimates

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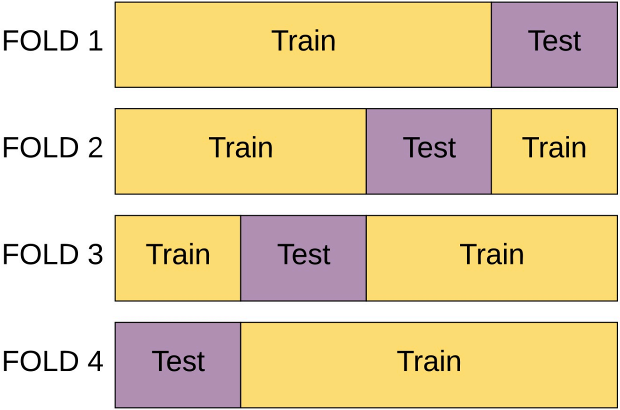
- **Challenge:** How to ensure systematic evaluation?
- May not use every data point for training or testing with random splits
- May be computationally expensive

# K-Fold Cross-Validation: Utilize Full Dataset for Testing



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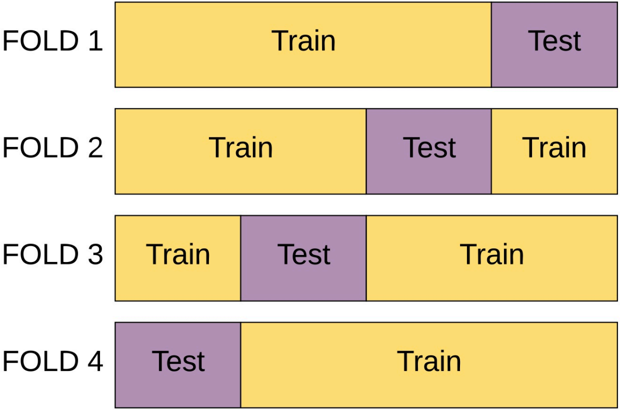

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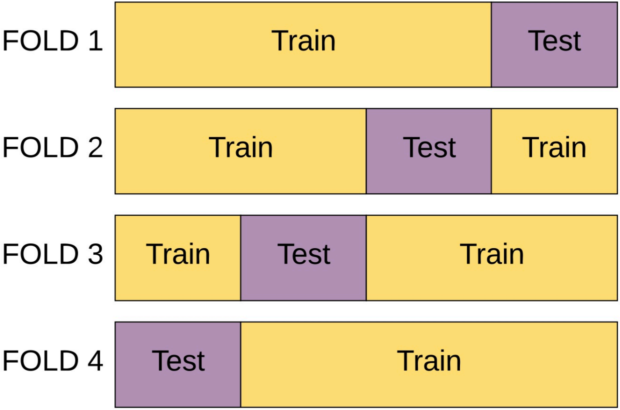

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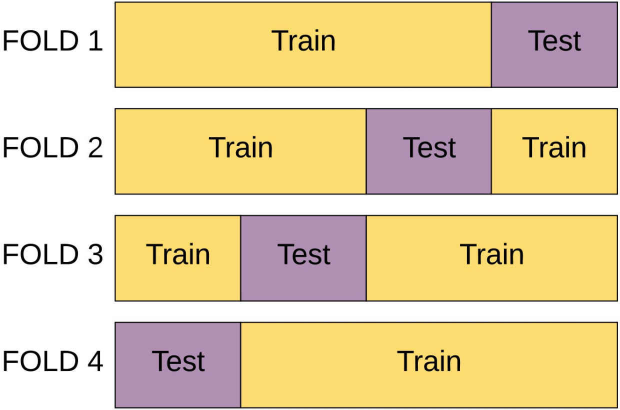

# Pop Quiz #8

**Question**

If you have 100 data points and use 5-fold cross-validation, how many data points are used for training in each fold?

# Pop Quiz #9

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# Pop Quiz #10

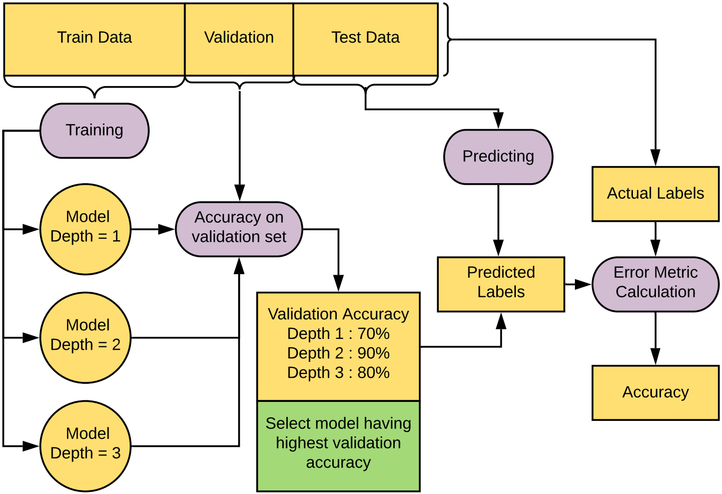
## Question

If you have 100 data points and use 5-fold cross-validation, how many data points are used for training in each fold?

## Answer

80 data points (4 out of 5 folds = $4/5 \times 100 = 80$)

# Optimizing Hyperparameters via the Validation Set



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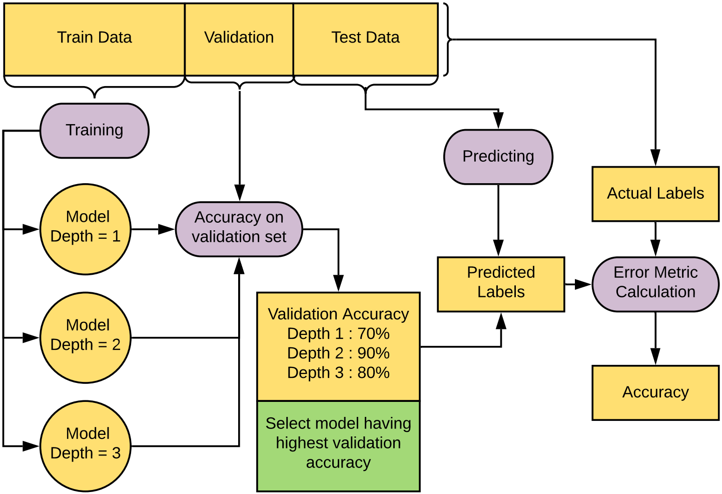

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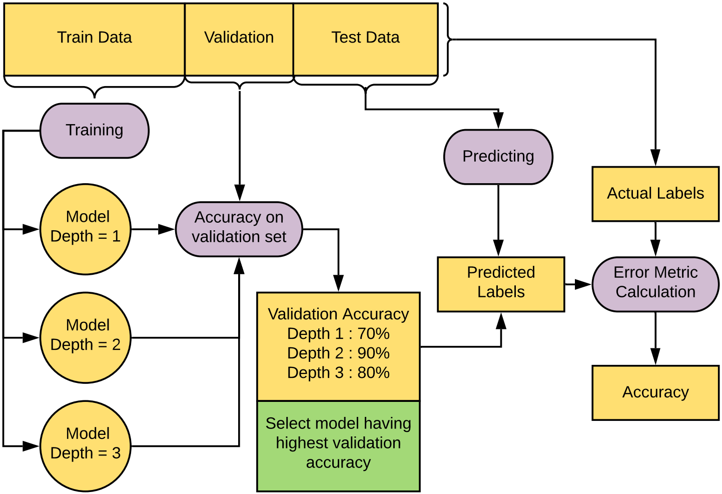


Validation set helps select the best hyperparameters

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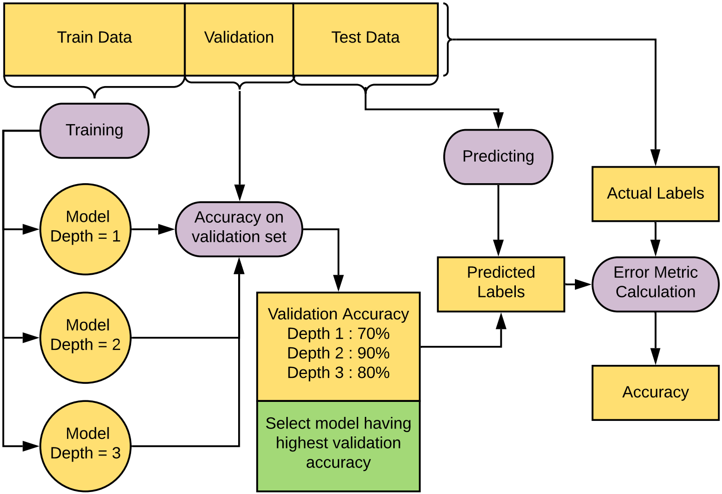


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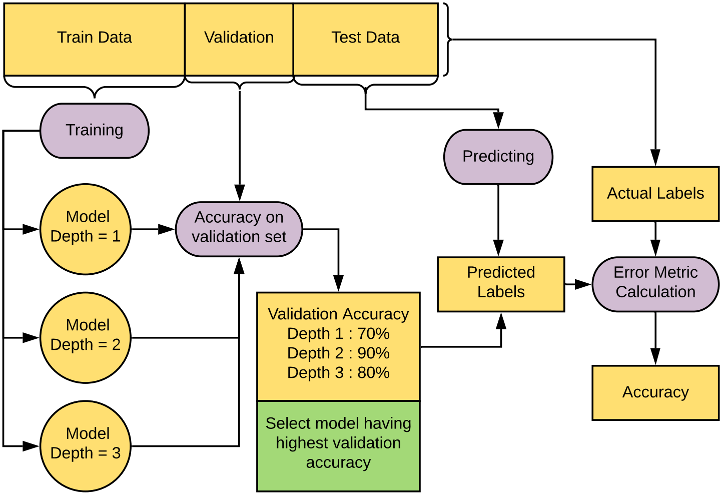

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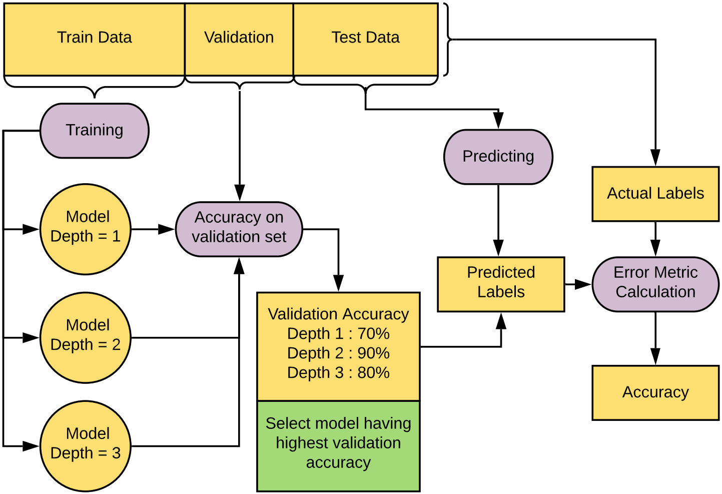


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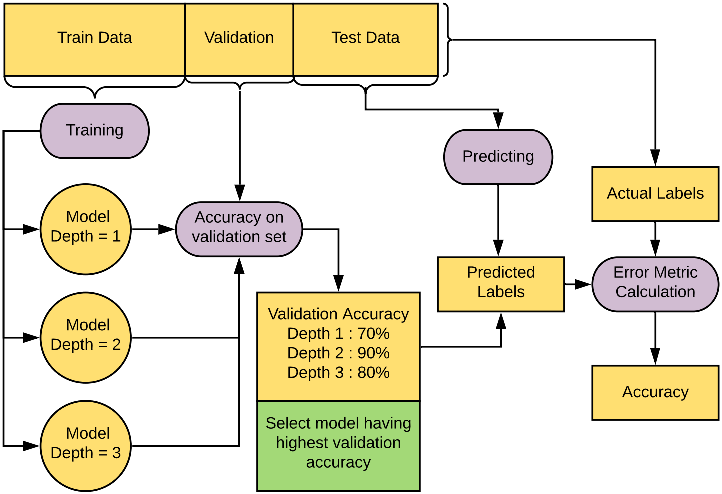
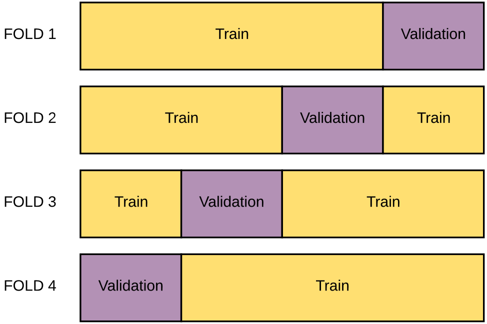



Validation set helps select the best hyperparameters

# Nested Cross-Validation Process

Divide your training set into *k* equal parts.
Cyclically use 1 part as "validation set" and the rest for training.
Here $k = 4$



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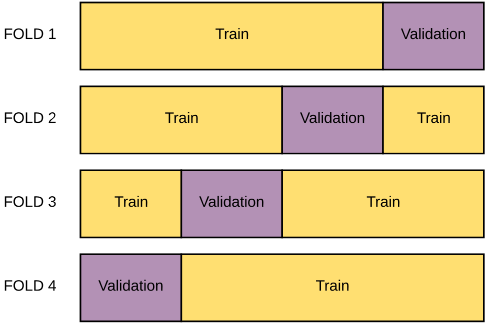

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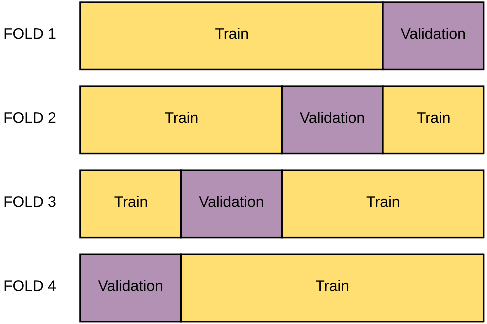


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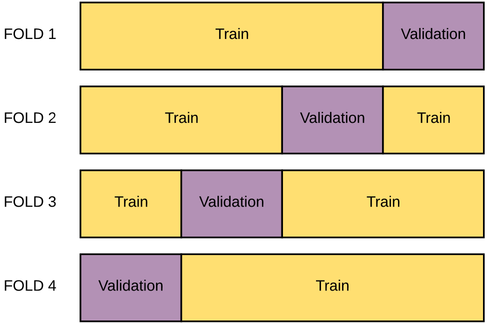


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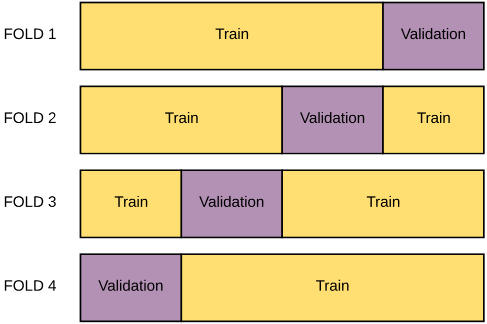


- Each fold provides one validation score
- Process is systematic and exhaustive

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**Question**

What is the difference between simple cross-validation and nested cross-validation?

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# Pop Quiz #13

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**Answer**

# Pop Quiz #14

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## Answer

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- Nested CV: Outer loop for model evaluation, inner loop for hyperparameter tuning

# Pop Quiz #16

## Question

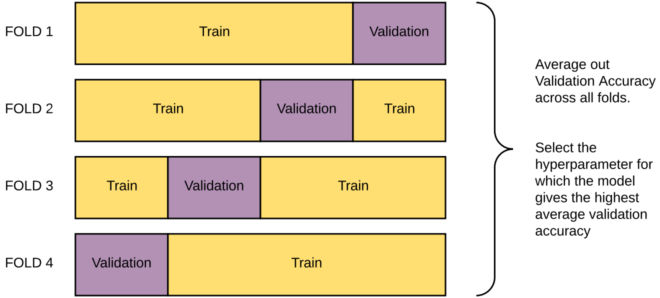
What is the difference between simple cross-validation and nested cross-validation?

## Answer

- Simple CV: Used for model evaluation only
- Nested CV: Outer loop for model evaluation, inner loop for hyperparameter tuning
- Nested CV provides unbiased estimates when doing hyperparameter search

# Cross-Validation Results

- Average out the validation accuracy across all the folds
- Use the hyperparameters with highest average validation accuracy



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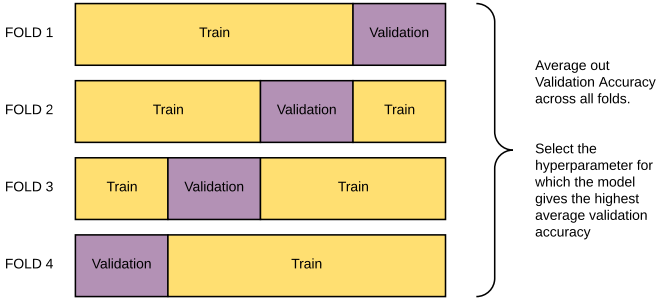

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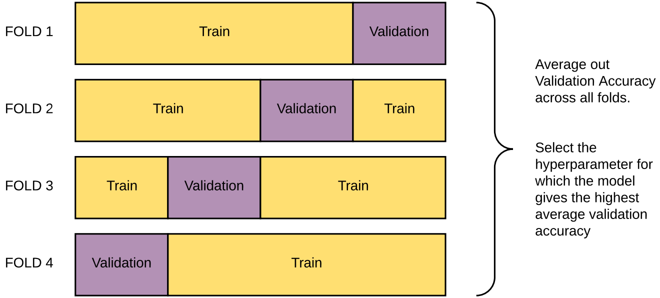


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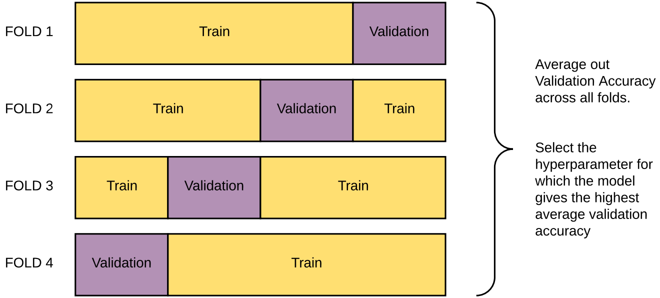


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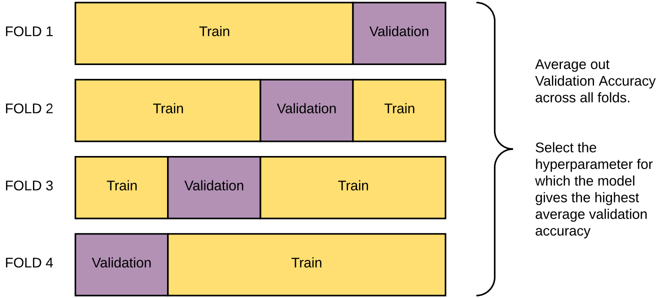


- Final model is trained on entire training set
- Standard deviation gives confidence in results

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Why do we average the results across all folds instead of picking the best single fold?

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# Pop Quiz #19

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## Answer

# Pop Quiz #20

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## Answer

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# Pop Quiz #21

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- Averaging provides more robust performance estimates

# Pop Quiz #22

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- Reduces impact of lucky/unlucky splits

# Pop Quiz #23

## Question

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## Answer

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- Averaging provides more robust performance estimates
- Reduces impact of lucky/unlucky splits
- Standard deviation indicates reliability of the estimate

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- Reduces variance in performance estimates

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**Question**

You have a binary classification dataset with 90% negative and 10% positive examples. Why is stratified cross-validation important here?

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## Answer

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# Pop Quiz #30

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## Answer

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- Stratified CV ensures each fold has $\sim$10% positive examples
- Results in more reliable and consistent evaluation

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- Time series data has temporal dependencies
- **Forward Chaining:** Train on past, test on future
- **Rolling Window:** Fixed-size training window
- **Expanding Window:** Growing training set over time
- Never use future data to predict past!

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- **Overfitting to CV:** Too much hyperparameter tuning
- **Wrong Preprocessing:** Scaling on entire dataset before splitting
- **Ignoring Class Imbalance:** Not using stratified CV when needed

# Pop Quiz #31

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What’s wrong with computing mean and standard deviation on the entire dataset before doing cross-validation?

# Pop Quiz #32

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## Answer

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- Test fold statistics influence the training preprocessing

# Pop Quiz #36

## Question

What's wrong with computing mean and standard deviation on the entire dataset before doing cross-validation?

## Answer

- This causes data leakage!
- Test fold statistics influence the training preprocessing
- Should compute statistics only on training folds

# Pop Quiz #37

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What's wrong with computing mean and standard deviation on the entire dataset before doing cross-validation?

## Answer

- This causes data leakage!
- Test fold statistics influence the training preprocessing
- Should compute statistics only on training folds
- Apply same transformation to corresponding test fold

# Pop Quiz #38

## Question

What's wrong with computing mean and standard deviation on the entire dataset before doing cross-validation?

## Answer

- This causes data leakage!
- Test fold statistics influence the training preprocessing
- Should compute statistics only on training folds
- Apply same transformation to corresponding test fold
- This gives more realistic performance estimates

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